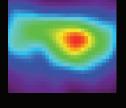




AUGUST 2011





Not So Permafrost Under Fire Viewport for Nuclear Fusion Hassle-Free Uranium

The Cell Membrane
Nature's Surprisingly
Active Doorway

Los Alamos NATIONAL LABORATORY EST. 1943

### 1663

LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

**About Our Name:** During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

About the LDRD Logo: Laboratory Directed Research and Development (LDRD) is a competitive, internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to our national interests. Whenever 1663 reports on research that received support from LDRD, this logo appears at the end of the article.

About the Cover: The membrane that surrounds a cell is a protective barrier that allows the cell to create

and maintain a life-sustaining environment, as well as a structural boundary that provides anchor points for the cell's internal skeleton and hundreds of different proteins. But, as discussed in the article on page 10, the cell membrane is also a functional element that can regulate the behavior of surface receptors and other proteins. Thus it is both rampart and sentry, doorway and gatekeeper. The cover illustration by Donald Montoya depicts this active cell membrane, about which we still have much to learn.



### Change at the Top

On June 1, Charles McMillan (bottom right) succeeded Michael Anastasio (bottom center) as director of Los Alamos National Laboratory. Shortly after McMillan was named director, he said, "I have great optimism for the future... The service we provide to the nation is just as important now as it ever was." Indeed, the rich history of the Laboratory goes all the way back to 1943, when the United States was struggling to turn the tide of World War II. The Laboratory's first director, J. Robert Oppenheimer (top left), led the staff in a successful effort to build the world's first nuclear weapons. Nuclear weapons brought the war to a rapid and decisive close, and played an important role in deterring aggression during the tenuous Cold War years. Following the Cold War, the nation ceased nuclear testing and the Laboratory entered an era of stockpile stewardship. Today, the Laboratory continues to apply science and technology to combat emerging threats to national security.

Top row, left to right:
J. Robert Oppenheimer,
director from 1943–1945
Norris Bradbury, 1945–1970
with incoming Director
Harold Agnew, 1970–1979
Donald Kerr, 1979–1986

Middle row: Sig Hecker, 1986–1997 John Browne, 1997–2003 Pete Nanos, 2003–2005

Bottom row: Robert Kuckuck, 2005–2006 Michael Anastasio, 2006–2011 Charles McMillan, 2011–



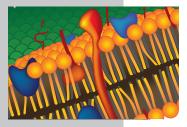
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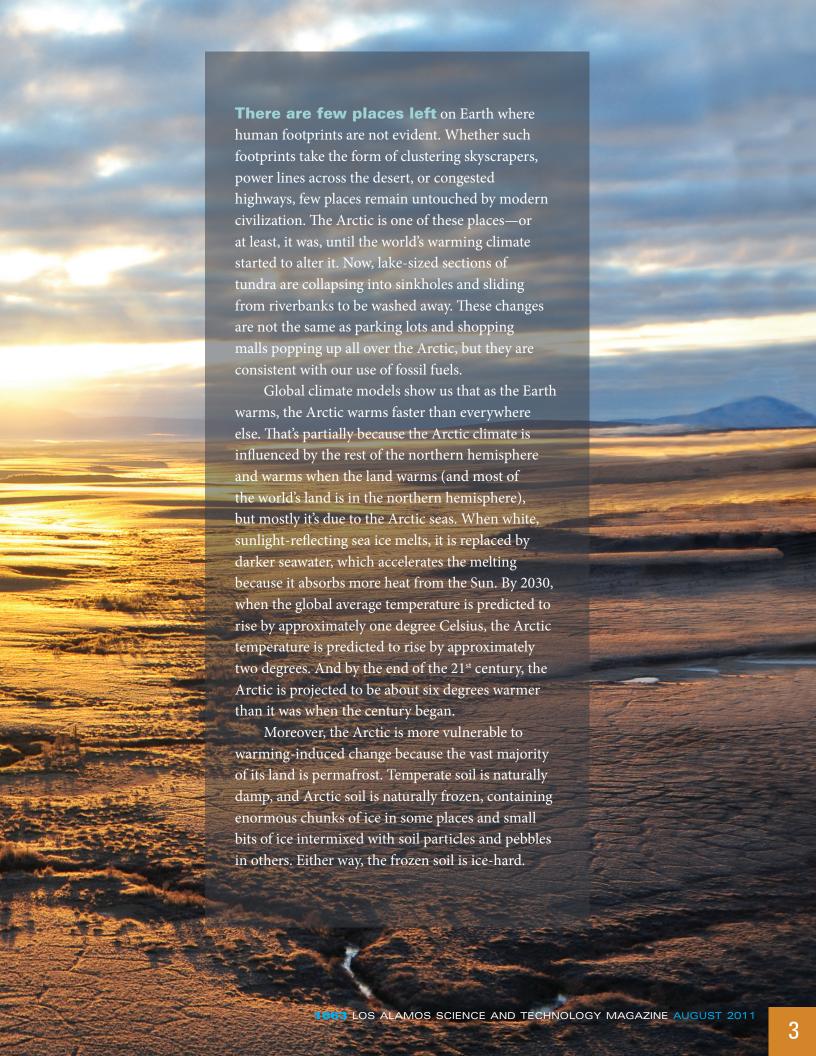


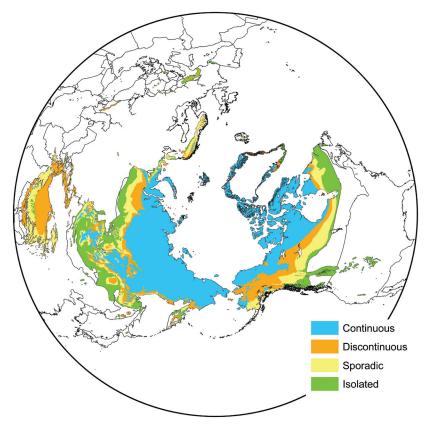
### **SPOTLIGHT**

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Most of the Arctic's continuous permafrost (blue) is likely to stay frozen as the climate warms throughout this century. Other areas are much more susceptible to thawing. CREDIT: NATIONAL SNOW AND ICE DATA CENTER, 2001

The term "permafrost" is reserved for any ground that has been continuously frozen, summer and winter, for the last two years (see map above). The longevity of permafrost is strongly influenced by not only its latitude, but also local factors, such as insulating vegetative cover or a north-facing hillside. Some tracts of permafrost have thawed and refrozen one or more times since a previous ice age, while other tracts remained continuously frozen for more than 100,000 years.

When permafrost thaws, there are serious impacts. Where large pockets of ice melt away, the ground collapses. On steep slopes, the surface soil slides away. Erosion patterns and water flows can change with the thaw, potentially accelerating the thaw rate. But the greatest impact of the thaw is underground, where bacteria and other microbes begin to multiply and migrate into the newly unfrozen soil. Bits of dead plant matter that have been safely stored in the frozen soil are now available for these bacteria to metabolize. The byproducts of that metabolism include carbon dioxide and methane—both potent greenhouse gases—and there's virtually nothing we can do to prevent these gases from reaching the atmosphere.

Estimates peg the amount of carbon stored in Arctic permafrost at a staggering 1.6 trillion metric tons. That's about twice the amount of carbon currently stored in the planet's atmosphere. Depending on how fast the permafrost

thaws, and how efficiently its carbon is released into the atmosphere, the rate of Arctic carbon released by bacteria could rival that from all human-made sources. And unless some counterbalancing phenomenon arises to save the day, such as plants and other organisms removing the excess carbon from the atmosphere, we are all but guaranteed a worst-case scenario from among the range of global warming projections. Thus, climate scientists want to know two things about the thawing Arctic permafrost: how much and how fast?

### **Under the Surface**

Permafrost soils reside just underneath the top layer of soil, known as the active layer. The active layer thaws every summer and refreezes every winter. In the northernmost reaches of the Arctic, the permafrost is hundreds of meters deep, underlying an active layer that's generally less than half a meter thick. Farther south, in the subarctic zone, 20–100 meters of permafrost typically support 1–2 meters of active layer. In some places, the full depth of permafrost has already thawed.

As the atmosphere gets warmer, the active layer warms up to the surrounding air temperature. This causes the permafrost underneath to thaw faster, partly because of conduction—the form of heat transfer that results when a warmer object (the active layer) is in direct contact with a cooler object (the permafrost just below). However, conduction is not the only way to transfer heat. There is also advection, which occurs when a fluid flows over an object. For example, a wind chill occurs when cold air flows over warm skin, causing heat to flow out of the skin and into the air. (Anyone who has ever experienced a wind chill knows how significant advection can be.) If a warmer fluid flows over a cooler object, the effect is reversed: heat flows from the fluid to the object.

In the case of thawing permafrost, advection comes into play whenever the permafrost makes contact with flowing water, such as groundwater. Even meltwater, with a temperature just barely above freezing, can transfer heat to the permafrost and increase the rate of thawing. So the fate of Arctic permafrost is not just a question of temperature, it's also a question of hydrology, the movement of water.

Consider, for example, any one of the many lakes found in the Arctic lowlands that occupy much of northern Canada, northern Siberia, and central Alaska. Only the upper two meters of the lake actually freeze in winter; the cold air can't freeze the deeper water. But the lake is nestled into

the surrounding permafrost, which has been frozen solid for hundreds of years, if not longer. It is perhaps somewhat counterintuitive that this arrangement—without moving water—is normally stable: The permafrost is unable to freeze the lake, because drawing heat from the lake would raise the temperature of the permafrost, rendering it too warm to draw more heat from the lake. Similarly, the lake is unable to thaw the permafrost, because transferring heat to the permafrost renders the lake too cold to heat up the permafrost any further. It is a delicate equilibrium that the warming climate threatens to disrupt. A very small increase in temperature could tip the balance, because even a trickle of meltwater is enough to bring advection into play.

As a result of the climate warming, perennially warmer lake water starts to thaw little pockets in the surrounding permafrost. Pores develop in the frozen soil. Over time, the pores link together into channels flowing with water. These channels, small at first, grow and multiply and potentially mingle with the flow of groundwater below. The slightly warmer lake water heats up the cooler groundwater, affecting

areas downstream. In this way, changes to the region's hydrology allow advection to degrade the permafrost much more rapidly than conduction alone.

In turn, damaged permafrost can lead to the formation of additional lakes. Whenever a large pocket of ice-rich permafrost collapses, it creates a depression in the ground known as a thermokarst. If that depression subsequently fills with water from surface flows, precipitation, or thawing permafrost, the result is a new lake, which could damage the surrounding permafrost further.

But warming lakes are not the only landscape effects of concern. For example, different depths of snow in winter and different types of vegetation throughout the rest of the year alter the insulating properties of the ground surface. As the Arctic landscape becomes warmer, the surface vegetation tends to shift from mosses to shrubs, and the full effect of this shift is not yet known. Because shrubs are darker than mosses, they absorb more heat from the Sun in summer, but they also shade and cool the ground. In winter, shrubs anchor a thicker and more insulating (warming) snow pack.



Thermokarst lakes form in the depressions that arise when large chunks of permafrost thaw, collapsing the ground surface. Past and present thawing episodes have left such lakes covering much of the Arctic landscape. Lakes and other surface water features can accelerate the damage to the underlying permafrost by creating pores and channels that could potentially connect to the groundwater below.

CREDIT: JOEL ROWLAND

But their dark, bare branches warm quickly and hasten the snowmelt, leading to less insulating (colder) ground conditions in the spring. Vegetation changes like this can begin with changing patterns of weather, erosion, and wildfire, all of which increase with a warming climate. In other words, a small increase in temperature could trigger a variety of processes—thermokarsts, erosion, changes in vegetation, lake-related advection, and others—to arise and contribute to the thaw.

### MAGHNUM, P.I.

At Los Alamos National Laboratory, a team of scientists is working to understand how local changes in hydrology might bring about major changes to the Arctic landscape, including the possibility of a large-scale carbon release from thawing permafrost. First, they must understand the local changes—from tiny, thawed pores in the permafrost to entire watersheds—before they can assess how the widespread occurrence of these local changes might become a planetary concern.

Bryan Travis, an expert in fluid dynamics, and Joel Rowland, an expert in hydrogeology and permafrostdominated river systems, are performing Laboratory-directed research and development to understand Arctic hydrology. Travis is author of the Mars global hydrology numerical computer model, or MAGHNUM, used for calculating heat and fluid transport phenomena. (MAGHNUM was previously used to model hydrological phenomena under freezing conditions on other planets, including Mars.) Travis advanced the MAGHNUM software with a variety of improvements and additional components into a new program, called ARCHY, a comprehensive Arctic hydrology model. Travis and Rowland work with Cathy Wilson, a Los Alamos scientist who specializes in predictive hydrology and geomorphology and heads up several Laboratory efforts on Arctic warming and climate. Together, the team's goal is to make ARCHY capable of accurately modeling Arctic

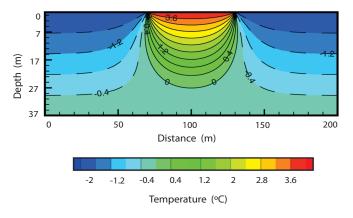
topography, thawing, and erosion. Because it includes advective heat transport, ARCHY will help to predict how quickly and how extensively the Arctic permafrost will thaw.

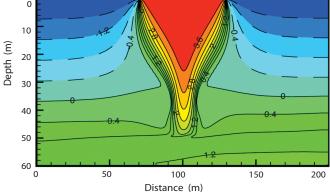
Travis has already used ARCHY to demonstrate the relative importance of advection. The figure below shows the predicted temperature gradients beneath an Arctic lake under two modeling scenarios. Without advection, 90 years of conduction leads to only minor thawing of the permafrost immediately supporting the lake. But when advective effects are included, the same 90 years is enough time for lake water to tunnel downward and connect with the groundwater flow, warming it by about one degree Celsius. The warmer groundwater then accelerates the demise of the permafrost downstream.

"What conduction alone would take a century to do happens in a few decades when advection is included as well," Travis says. Wilson adds, "It's clear that these hydrological processes need to be represented in the next generation of climate models if we hope to predict the impact of climate change on the rates of permafrost thaw and carbon release in the Arctic."

ARCHY must also be able to apply its thawing predictions to the bacterial processing of carbon in the permafrost. This, too, adds interesting and important complexity to the problem. Some bacteria metabolize carbonrich matter in the soil aerobically—making use of oxygen from the air. They convert organic forms of carbon in the soil to carbon dioxide ( $\rm CO_2$ ), which can then enter the atmosphere. Other bacteria are capable of converting organic carbon into methane ( $\rm CH_4$ ) under anaerobic conditions, such as when the soil is so damp as to limit the available oxygen. Both  $\rm CO_2$  and  $\rm CH_4$  are major greenhouse gases, but  $\rm CH_4$  has a substantially greater warming effect; therefore, it is important to know the ratio of the two emission rates.

Because the emission of  $\mathrm{CH_4}$  results from an aerobic processes in wet, oxygen-deprived soils, it is enhanced by





Computer modeling reveals the importance of the advective—that is, fluid-flow-based—mode of heat transfer. Each frame shows an underground vertical slice through the same Arctic lake embedded in the permafrost after 90 years of simulated time evolution. The simulation on the left allowed only conductive heat transfer—no moving water. At right, water was allowed to flow through thawing soil pores, inducing advective heating. With advection, the lake water reached the groundwater, flowing right to left about 50 meters below the surface, and more rapidly thawed the surrounding permafrost. The numbers on the axes are distances in meters, and the color scale spans temperatures from -2 (blue) to +4 degrees Celsius (red). The liquid-solid (unfrozen-frozen) boundary in both frames is the solid, zero-degree contour line. Dashed contour lines indicate below-freezing temperatures.







Top: Patterned ground appears where large ice wedges form beneath cracks in the surface soil. These cracks widen whenever surface water enters the cracks and then freezes. But with climate warming, the water takes longer to freeze, allowing enough time for the ice wedges below the cracks to melt. This leaves a void into which the surface soil collapses. Water gathers in the collapsed depression and accelerates the thaw.

Middle: Retrogressive thaw slumps, like this one along Alaska's Selawik River, form when thawing permafrost weakens the land, causing it to slump as the former terrain runs off into the river. The exposed soil at the top of the slump is thawing now, and will probably break away again. At other sites, this cycle has been observed to repeat for up to 50 years, widening up to a kilometer from the riverbank.

Bottom: The rate of riverbank erosion in temperate and tropical climates is primarily determined by the water flow rate, with larger flows washing away more soil. However, the rate of erosion of an Arctic riverbank, like this one along Alaska's Yukon River, is primarily determined by the water temperature, with warmer water causing more damage to the permafrost underlying the active layer.

rain (which is predicted to increase with global warming) and watery surface conditions. If, in addition, thawing creates more bogs and swamps, the greenhouse gas ratio will include more  $\mathrm{CH_{4}}$ . The ratio will also vary seasonally, because some anaerobic metabolism continues even under partially frozen conditions, while aerobic metabolism does not. All of these processes must be accounted for if ARCHY's output is to accurately capture the Arctic's effect on global climate change.

### **Visible Changes**

Evidence for the big thaw is already written large throughout the Arctic landscape.

In addition to thermokarsts and other varieties of collapsing land, much of the Arctic is characterized by patterned ground (see top photograph), where large subsurface ice wedges form the boundaries between segments of soil shaped like polygons. These features form in regions where the active layer and permafrost shrink and crack under cold winter temperatures. In the spring, surface water seeps into the cracks and freezes in the still-frozen permafrost. Because water expands as it freezes, the original crack must widen each time new water is frozen into it. When climate conditions warm, the temperature of the shallow permafrost is too high to quickly freeze the new water, and the ice wedges below start to melt. Eventually the soil over the melted ice wedge collapses, forming warm ponds that cause even more permafrost thaw and ice wedge melt.

Perhaps the most striking landscape change occurs when enormous chunks of land disappear entirely. On the moderately steep banks of the Selawik River in Alaska, for example, Rowland studies a phenomenon known as a retrogressive thaw slump (see middle photograph). The

Should it prove critical to slow down the thaw, Cathy Wilson, Joel Rowland, and Bryan Travis are holding on to a last-ditch option.

thawing permafrost destabilizes the ground, causing it to break off and slide downhill into the river, whose current carries the soil downstream. It is retrogressive because it progresses backwards: permafrost left behind after a slide is suddenly exposed, rendering it vulnerable to faster thawing and destabilization. The thawing land continues to break off and slide away, year after year. How far it progresses and what causes it to eventually cease are not yet known. The Selawik slump,

meters every year since.

"Beyond the obvious effect on the local hillside, the impact of a retrogressive thaw slump can be felt throughout the river system," Rowland points out. "When that much sediment is added to a river system all at once, there can be important consequences downstream." Indeed, the runoff from the Selawik slump flows downriver to a fishery. If too much sediment from the slump accumulates in the fishery, it affects the river's sheefish population. Like salmon, sheefish need clear, sediment-free water to oxygenate their eggs, so a

for example, started in 2004 and has receded about 15 to 20



murky river bottom threatens not only a fish population, but a local village's livelihood as well.

Additionally, river currents can deposit excess sediment as new sandbar islands in the middle of the river. The warming climate favors the rapid colonization of these islands by shrub vegetation, which tends to stabilize the soil and give the islands some permanence. The islands constrict and accelerate the river's flow. While earth scientists see no particular catastrophe as a result of this, they do expect some outcomes—affecting boat navigation, fish habitats, and nutrient loads, for example—even far downstream where the river meets the ocean.



This 2009 satellite image of Alaska's largest river, the Yukon, has been overlaid with the same stretch of river as it appeared in 1974. By comparing the river's recent location (lighter blue) with its location 35 years earlier (darker blue), one can observe the river's migration and a new population of vegetated islands, spawned by the increased sediment deposition from the destabilization and erosion of permafrost upstream.

SATELLITE IMAGE COURTESY OF GEOEYE



Arctic rivers are experiencing other changes, too. Rivers naturally migrate over time, shifting locations as their riverbanks erode. (See bottom photograph, page 7, and satellite image, page 8.) Rowland and others have found that river migration in the Arctic, unlike that in other regions, depends more on the temperature of the water than its flow rate because Arctic riverbanks are made of permafrost, which must partially thaw before they can be significantly eroded. So global warming is likely to increase the rates of Arctic river migration and floodplain erosion, and thereby provide additional mechanisms for releasing long-frozen carbon into the atmosphere and oceans. Thus, river migration and other sediment redistribution processes join the list of Arctic climate phenomena that Los Alamos scientists seek to understand and ultimately predict.

### **Northern Blights**

Computer models predict global climate change by breaking the world's land, sea, and atmosphere into manageably small blocks—but not so small that the computers can't juggle them all. Unfortunately, the scale of the Arctic hydrological changes in progress—to lakes, rivers, and underground flows—is often much smaller than a single block. How, then, can the Arctic's important hydrological effects be incorporated into global models? How can one aggregate a widespread pattern of collapsed and fractured ground? What thawing effect can be expected from a cluster of a thousand lakes? Arctic researchers at Los Alamos are studying various Arctic phenomena to address these questions. Success will mean characterizing all the small-scale changes in a way that can be accurately and conveniently represented on the global scale.

The Los Alamos researchers are deploying sensors and reviewing other data to address many pieces of the overall puzzle—pieces that will be assembled in the next few

Data from instrumentation on the ground and in space are needed to constrain the range of climate and landscape changes expected above the Arctic Circle. Computer-based algorithms mine satellite images for subtle signatures of widespread change in the Arctic. Images like this one of the many lakes of the Lena River delta in Siberia help researchers to identify changes over time and their impacts on local hydrological patterns. Inset: This ground-based sensor system measures rainfall, solar radiation, air temperature, humidity, soil temperature, and soil moisture.

CREDITS: (LEFT) LANDSAT IMAGERY COURTESY OF NASA GODDARD SPACE FLIGHT CENTER AND U.S. GEOLOGICAL SURVEY, (RIGHT) JOEL ROWLAND

years. Will a thawing region tend to deform in a way that concentrates the surface water into streams, thereby drying out the rest of the landscape? Los Alamos is examining this with high-resolution topographical data obtained by lidar, a laser-reflection measurement system. Will lakes expand and merge with more meltwater, or will they drain through underground channels into the groundwater? Los Alamos is addressing these questions by training a sophisticated computer algorithm to recognize the changing surface water distribution in satellite imagery of the lake country (above). Such information, once aggregated, will be used to inform and improve scientists' understanding of the global climate.

The degree of surface damage the Arctic will ultimately suffer is not yet known. How much carbon its thawing permafrost will release into the atmosphere and how soon it will happen are not yet known. It's not even clear that the carbon release poses a problem; perhaps the Arctic ecosystem will surprise us with some way of consuming it. What is clear is that the Arctic temperature is rising, its permafrost is thawing, and its surface is crumbling. Scientists have observed a 200 percent increase in surface scars (thermokarsts, active layer erosion features, and thaw slumps) over the last 25 years. The Los Alamos work helps link these changes into a deeper understanding of the global climate system. �� LDRD

—Craig Tyler



## Surprisingly active Understanding the Cell Mem-

Far from being static barriers, the membranes that nature uses to separate one environment from another are dynamic structures that, if understood, could help us take better care of our cells and ourselves.

Jarek Majewski of the Lujan Neutron Scattering Center at Los Alamos used to be completely focused on material interfaces, the vanishingly thin boundary regions where two materials—a gas and a liquid, a liquid and a solid, two solids, etc.—meet and find ways to get along. And he's still focused on that thin interface, except increasingly, Majewski finds he's drawn to organic interfaces and the remarkable biological membranes that often serve as life's boundaries.

Biomembranes surround living cells (cell membranes), cordon off the cell nucleus (nuclear membranes), line the lungs, coat nerve fibers, and form vesicles or cavities within cells. Just a few tens of atoms thick, they are nonetheless strong and tough, somewhat akin to a resilient soap film, if one could imagine such a thing. This soapy film is simultaneously structural and functional, serving as both doorway and gatekeeper for molecules that enter or leave a cell, and as anchor and regulator for surface proteins. But while their existence was confirmed more than a century ago, biomembranes remain some of the least understood components of living systems. To Majewski, they are as compelling as a red carpet is to a Hollywood starlet.

"We know that these membranes contain cholesterol," he begins to explain, "and if they absorb just a little more, or if sugar molecules are added to the local environment, there can be a huge change in the biomembrane's stiffness and other mechanical properties. For most biological systems, structure and function are interrelated, so altering a cell membrane's structural properties likely results in changes in cellular functions."

And changes in function could be disastrous. For example, consider that when we breathe, nearly half a billion air sacs (alveoli) in our lungs expand and contract, forcing the exchange of carbon dioxide and oxygen across the alveoli's flexible walls. Those walls are coated with a liquid that, on the one hand, helps the gases diffuse into and out of a wall, but on the other, has a surface tension that tries to reduce surface area and so hinders the wall's expansion.

We're able to breathe because the alveolar membrane (also called lung surfactant)—a monolayer of proteins and small molecules called lipids—forms the interface between the air and liquid. The membrane reduces the surface tension enough that the air sacs can expand. Insufficient levels of lung surfactant, found in either premature infants or in adults suffering from disease or trauma, can result in respiratory distress syndrome, a potentially lethal disease in both populations.

Majewski continues, "Changing the sugar concentration around the alveolar membrane would change its flexibility, which would dramatically affect alveoli function. So where in the body is the sugar concentration the most carefully regulated? In the lungs. It's fascinating."

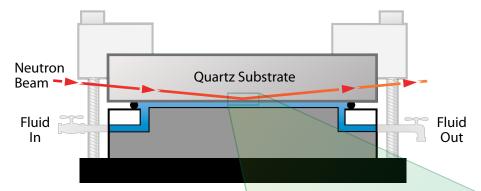
### **It Takes a Neutron**

Biomembranes come in two common forms, monolayer and bilayers. (A bilayer is simply two monolayers arranged belly to belly, as in the Figure on page 13.) Surprisingly little is understood about the details of how they function in the body because, well, there just isn't enough to them to study.

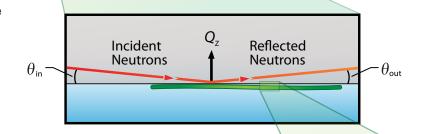
With a thickness of roughly one-hundredth the wavelength of visible light, biomembranes are too thin to be resolved by an optical microscope—there is no hope of seeing a cell membrane in action. Furthermore, biomembranes only function in an aqueous environment, but water scatters visible and ultraviolet beams of light, so return signals are swamped by water-induced background. Watery environments also limit the utility of electron microscopes, because electron microscopy typically requires the sample be in vacuum.

Different problems confront researchers who try to shine x-rays on the subject. X-ray diffraction techniques work best when probing ordered atomic structures, so the usual way for researchers to obtain a diffraction signal is to make a crystal from whatever they want to probe. But biomembranes don't form crystals. They remain as individual

Neutron reflectometry is a technique that can provide detailed information about a biomembrane. The membrane is prepared on a substrate, such as a flat piece of quartz, and placed within a chamber where the temperature, pressure, pH, etc., are controlled. The chamber is positioned such that a highly collimated beam of neutrons



hits the membrane at a slight angle  $\theta_{\rm in}$ . The researcher measures the intensity of those neutrons reflected from the membrane at the angle  $\theta_{\rm out} = \theta_{\rm in}$ . Because the neutrons change direction, they change their momentum perpendicular to the membrane surface by an amount  $Q_2$ . With the reflectivity R defined as the ratio of the incoming neutron intensity to the reflected intensity, the shape of the R vs.  $Q_z$  curve provides detailed information about the membrane.



monolayers or bilayers, neither of which have enough layers of atoms in thickness to provide a standard diffraction signal. Biomembranes don't scatter x-rays particularly well, either, because the ability of an atom to scatter x-rays is proportional to how many electrons it has, and biomembranes are principally made of light atoms, such as carbon, oxygen, and hydrogen, which have relatively few electrons.

It turns out that neutrons, the electrically neutral particles that rub elbows with positively charged protons in the atomic nucleus, make some of the best probes for biomembranes. Neutrons scatter or reflect cleanly from the atoms in a membrane and (unlike x-rays) don't cause damage; plus, the chargeless neutrons pass effortlessly through the thick substrates used to support thin membranes during experiments. Most of all, researchers now have experimental techniques to eliminate neutron signals arising from interactions with the water, while recording the signal from the lipids or proteins, making the membrane "visible" within its watery environment.

Neutron studies require lots of neutrons, and the Lujan Neutron Scattering Center at Los Alamos has one of the most intense sources of neutrons in the world. The international user facility hosts more than a dozen large-scale instruments, each designed to exploit different types of interactions between neutrons and matter. Majewski works primarily with the surface profile analysis reflectometer (SPEAR), one of the Lujan Center's workhorse instruments that can study even the thinnest organic and inorganic layers in a variety of environments.

Collaborating on several fronts with colleagues

from the United States and abroad, Majewski has embarked on an ambitious research program to better understand the structure and function of biomembranes and biointerfaces. He's taken a systematic, bootstrap approach, learning first how to create simple artificial membranes that have some of the properties of real biomembranes, then learning how to optimize the use of SPEAR or other instruments to obtain ever more detailed information. By comparing his data to simulated output, he can interpret how his surrogate membranes behave as a function of local conditions.

Majewski then uses what he's learned to create more realistic biomembranes; increase the sophistication of his experiments, his data collection methods, and data analyses; and improve his theoretical models. It's the scientific method at its best.

His efforts have begun to pay off on several fronts. For example, with his collaborators, postdocs, and students, Majewski recently used a technique known as neutron reflectometry to probe the adhesion of mouse fibroblast cells to a solid substrate. This experiment was the first demonstration that neutron reflectometry could be used to study a living colony of cells. The team hopes to advance the understanding of how cells adhere to vascular walls and implants, with a goal of preventing thrombosis—the formation of blood clots.

But Majewski is a type-A experimentalist who seems to be investigating virtually anything that has to do with biomembranes and biointerfaces. He's looking into polymers that seal holes in the membranes to prevent cell leakage (the

Facing page: An artist's conception of a cell membrane shows a bilayer of lipid molecules (green heads, yellowish tails) studded with proteins (various shapes and colors). The orange sections represent lipid rafts, which are areas of higher lipid density that attract and concentrate certain proteins. The lipid density of a raft affects the function of any embedded proteins, suggesting that the cell membrane might play an active role in regulating protein function. The inset shows a phospholipid.

A typical neutron reflectivity R versus momentum transfer  $\mathcal{Q}_z$  curve for a thin film layered on a flat quartz substrate. The location, shape, and amplitude of each bump and wiggle depends on the thickness, density, and roughness of the thin film.

holes are created on a massive scale following a powerful electrical shock), novel antimicrobial peptides that will dissolve bacterial membranes, antioxidants to protect membranes from attack by oxidative molecules, the interaction of membranes with heavy-metal salts, the biophysics of wrinkling, and the role played by cholesterol in the cellular membranes.

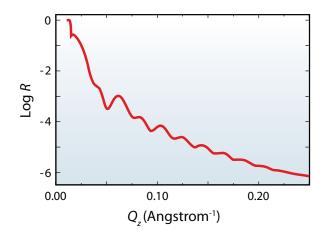
The mouse fibroblast experiments, however, are significant because they mark a radical departure from the smooth samples and simple models that were experimental and theoretical necessities in the past. The experiments cracked open the door to exploring complex, experimentally messy living cells under somewhat natural conditions.

### **Lipid Molecules**

A biomembrane's properties derive largely from the interactions of phospholipids. Phospholipids, and lipids in general, are small molecules that have a "head" region coupled, tadpole-like, to a "tail" of one or more hydrocarbon chains. The head group is polar: electrons are distributed unequally about the head, creating an electric field that can attract or repel other polar molecules (or ions). The tail is made from electrically neutral chains of primarily carbon and hydrogen atoms—the molecules from which oil and wax are made. While the lipid head is quite comfortable being surrounded by other polar molecules, such as water, the tail likes to be in oil and avoids water like the plague.

In a watery environment, phospholipids can spontaneously arrange themselves so as to make both parts of each molecule happy. Depending on conditions, they can assemble into several possible configurations, one of which is the bilayer membrane. The heads interface with the water by forming the top and bottom surfaces of the membrane, while the tails, sandwiched between the two surfaces, revel in their self-made oily surroundings.

A cell membrane is usually made from several kinds of phospholipids and scores of different proteins adorning both

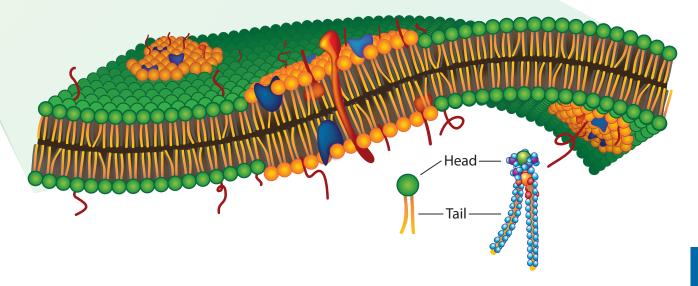


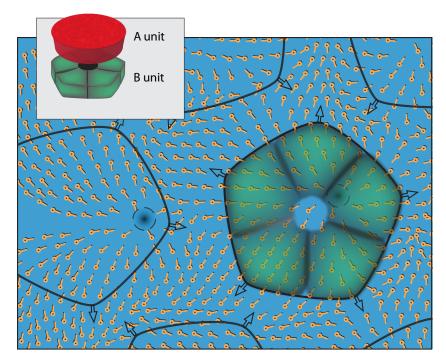
surfaces or poking through the membrane from one surface to the other. The proteins serve as receptors for other proteins or small molecules, as communication towers, or as gateways controlling the flow of nutrients and other molecules into and out of the cell. More than 30 percent of the proteins encoded for in our genome are integrated with the cell membrane, while more than 60 percent of all drugs interact with the membrane-bound proteins.

### **The Active Cell Membrane**

It seems odd that a structural boundary would be active, changing its mechanical properties as its environment changes (imagine your living room walls becoming more flexible as the room heats up), but the cell membrane does just that. A broad range of lipid-lipid and lipid-environment interactions causes the membrane to assume different physical phases, ranging from a low-density, liquid-like state to something more tightly packed and gel-like. The phase depends on the local conditions (surface pressure, temperature, pH, etc.) and the membrane's complement of lipids and proteins.

A structurally active boundary begins to make sense with the knowledge that several phases can coexist within a single membrane. In particular, tightly packed nanodomains, or lipid "rafts," float within a liquid phase. The rafts are assembled from select lipids and are heavily populated with specific proteins—to the exclusion of other lipids and proteins.





Cholera toxin is a protein complex that infiltrates the cells that line the small intestine. The complex (inset) consists of the B unit, which anchors the protein to the cell membrane, and the toxic A unit. Once it passes through the membrane, the A unit causes the cell to release water, and overall the body dehydrates. Computer simulations reveal what happens to the lipids in the membrane when the B unit binds. In the large illustration, the black arrows show direction and tilt of the GM1 receptors (see text). The orange symbols depict the conformations of the lipids forming the membrane. The binding of the toxin introduces a whorl (outlined circle), or a depression in the membrane that could trigger the A unit's entry into the cell.

The cell's dynamic membrane becomes a thing of beauty, however, with the realization that the membrane can influence the structure and function of embedded proteins, while in turn, proteins can impact the organization of the lipids surrounding it. Suppose the cell membrane becomes, say, less rigid and more fluid in response to a change in the chemical environment outside the cell. Then the behavior of various proteins embedded in or through the membrane can change and potentially modify processes that the cell uses to change its chemical surroundings.

"Cells respond to their environment," says Majewski. "So it's quite possible that the cell uses its membrane to regulate its own behavior."

### The Texture of Cholera

The direction of Majewski's research changed decisively about eight years ago, when he became one of the principals of a collaboration focused on understanding how cholera toxin enters a cell.

Cholera can result if a person's intestine becomes infected with the bacterium *Vibrio cholerae*. Approximately 1 in 20 infected persons become severely ill and suffer intense watery diarrhea, vomiting, and leg cramps. The rapid

loss of body fluids leads to dehydration and shock, and without treatment, a painful death can occur within hours of infection.

The toxin itself is a large protein in six parts: a B unit comprising five identical subunits arranged in a five-sided ring with a central hole, and a bulky A unit that sits above the hole in the B ring. The toxin attacks the cell by docking with certain receptor molecules made from ganglioside glycolipid (GM1 receptors), which are frequently found in lipid rafts on the membrane surface. Only after the ring is docked will the A unit detach and pass through the hole in the B ring, enter the cell, and wreak havoc.

Lipid molecules in the raft are densely packed, and passing the bulky A unit through the membrane seems as unlikely as landing a jetliner in a dense forest. So it is natural to ask how it happens. A similar question could be asked for an entire group of toxins that are structurally similar to cholera toxin, including the neurotoxin botulinum, which is responsible for botulism illness, and the heat-labile enterotoxin, responsible for that bane of the world traveler, "Montezuma's Revenge."

Majewski, collaborating with Tonya Kuhl (from University of California, Davis), Chad Miller and Erik Watkins (from University of California, Davis, and the Lujan Center) developed new techniques in neutron reflectometry and advanced two x-ray techniques that yield information about surfaces—grazing-incidence x-ray diffraction (GIXD) and x-ray reflectometry—to study the mechanism by which cholera's B ring binds to GM1.

Using their own newly developed artificial membranes, the collaborators showed that each of the five subunits of the B ring grabbed a GM1 lipid, so that five receptors were pulled toward each other, creating a sturdy compact domain within a lipid raft. In 2006, they hypothesized that such an action could trigger endocytosis, wherein the membrane beneath the toxin infolds and forms a cavity within the cell. The membrane would hold onto the toxin as it collapsed and, like quicksand, suck the toxin into the cavity.

It was evident, however, that docking to the GM1 receptors distorted the lipids comprising the raft. The lipid tails typically run perpendicular to the membrane surface like the crewcut hairs on a marine sergeant's head, but the



The SPEAR instrument is a neutron spectrometer and one of the premier tools for measuring the properties of thin films. Researchers from around the world come to the Lujan Center to use SPEAR (logo at lower left). Shown in the photo are SPEAR users (left to right) Peng Wang, Jarek Majewski, Saurabh Singh, and Manish Dubey.

research team found the tails "tilted" and stretched out at an angle. This thinned the lipid bilayer, and it was noted that the tilted tails were likely to stress the membrane and cause it to undergo a phase change, and perhaps that's what allowed the toxin to breach the boundary.

As the years rolled by, Majewski's team was able to evolve their equipment and measurement techniques. The result was their application of GIXD to obtain information of unprecedented detail about the way in which the lipid bilayer distorts in response to the binding of cholera toxin. In a paper published recently by the Proceedings of the National Academy of Sciences, the group showed that the toxin introduces a cowlick into the membrane, a whorl created by the binding of the five B subunits to five GM1 receptors, as can be seen in the figure on page 14. The center of the whorl is a physical anomaly, a depression or weak spot that may trigger endocytosis.

Interestingly, the team learned that binding of the toxin to lipid receptors does stress the raft, which does change phase, only into an unanticipated, previously unobserved structural phase. This "texture" phase, as it's called, is characterized by the particulars of the tilted tails and by a lipid density that lies midway between the known low-density liquid phase and a high-density gel-like phase.

Although the exterior-facing raft layer experiences the stress directly and changes phase, van der Waals forces cause the lipids of the interior-facing layer to enter a texture phase as well. Proteins embedded in the raft in either layer could alter their behavior. Majewski speculates that the texture phase may enable a new type of membrane-only signaling for the cell, where "information" from outside the cell is translated by way of the tit-for-tat phase transition, into a change of protein behavior inside the cell. Any new signaling mechanism would represent a new opportunity to understand the workings of the cell.

### **A Source to Forget**

The exuberant Majewski is unexpectedly deferential as he mentions what could be life-changing results from new experiments.

"You've heard of the correlation between lipids and Alzheimer's disease?" he asks. "There's still much conjecture



about the reason for the correlation. We may have found something along those lines that is very significant."

Alzheimer's is the life-robbing loss of memory that currently afflicts more than 5 million people in the U.S. When an Alzheimer's victim's brain is examined postmortem, hard, insoluble deposits known as plaques are found distributed throughout. The plaque is made from tiny pieces of unwanted protein called beta-amyloid, and although beta-amyloid's presence in the brain is correlated with the disease, the relationship is unclear.

Majewski's team and his collaborator Ka Yee Lee from the University of Chicago have shown that certain lipids with negatively charged head groups tend to attract beta-amyloid. Those lipids are typically found on the leaflets of the bilayer membrane facing the interior of the brain cells, but Majewski recently participated in experiments that proved the membrane can somehow bring the special lipids to the exterior layer. There, they can provide a favorable binding site for beta-amyloid that allows plaques to grow. It's then possible that a person in whom these lipids are produced and more easily transported to the exterior membrane would be at higher risk for Alzheimer's disease.

Whatever the future holds by way of biomembrane research, Majewski knows that he's found a field of study worthy of a life's work. The membranes are fascinating, little is known about them, and the research has the potential to change people's lives. But he admits that part of his fascination stems from a frontiersman's sense of a challenge. "So little is known about biomembranes that at some point during the research, you realize you're on your own, that you've wandered into terra incognita. That's when it starts to get really interesting." •

—Jay Schecker

# UNDER FIRE



Stephanie Windle from the La Grande, Oregon, branch of the interagency hotshots, an elite wildfire crew, spent two weeks fighting the Las Conchas blaze. CREDIT: KRISTEN HONIG/U.S. FOREST SERVICE

### On June 26, 2011, a tree downed a power line,

igniting a fire near the Las Conchas trailhead deep in the Jemez Mountains of northern New Mexico. The region had not received significant precipitation in nine months, and the combination of a parched landscape with unpredictable, gusty winds was a recipe for disaster.

Residents from towns surrounding the blaze watched the plume rise as the fire consumed the forests and grasslands. Fanned into a conflagration by the gusting winds, the fire burned 43,000 acres in a dozen hours, almost tripling in a few days to become the largest in the state's history. It reached the edges of Los Alamos, a community of 18,000, and skirted the perimeter of the town's namesake national laboratory.

The Las Conchas fire aroused public concerns that nuclear or other hazardous materials stored on Laboratory property—plus Cold War-era contaminants in the surrounding canyons or forests—could become exposed to the environment and migrate downstream or be released into the air. Watersheds were also burned, leading to concerns of flash floods, severe runoff, and erosion during the July and August monsoon season.

The Laboratory, however, was well prepared to address such concerns, in no small part because of some hard lessons learned more than a decade ago. In May of 2000, the Cerro Grande Fire burned a 47,000-acre scar across the Jemez into Los Alamos—destroying hundreds of homes in addition to



structures at the Lab. Since then, the Laboratory has improved fire-protection systems sitewide. It built a multiagency Emergency Operations Center and an interagency fire center with a helicopter base and water dip tanks onsite. It removed massive amounts of fuels, improved fire breaks and roads, improved storm runoff and erosion controls, planted vegetation and structures to help prevent contaminants from flowing down canyons, and provided new equipment and training for the community's fire department.

The planning and hard work paid off. As stated by Laboratory and government officials, all hazardous materials—including any at waste and environmental remediation sites—were safe, accounted for, and protected.



Crews from across the West manage lines above Guaje Canyon, north of Los Alamos. CREDIT: KRISTEN HONIG/U.S. FOREST SERVICE

The fire consumed vast parts of Valles Caldera National Preserve; expansive private land, including the Pajarito ski area; and 60 percent of Bandelier National Monument, with its prehistoric artifacts. The blaze scorched four Native American Pueblo territories and displaced residents for weeks.

6/26 6/27 6/28 6/29 6/30 7/1 7/2 7/3 7/4 7/5 7/6 7/7 7/8 7/9 7/10 7/11 7/12 Santa Clara Valles Caldera National Preserve os Alamos Los Alamos National Laboratory Bandelie Jemez Pueblo

While the Las Conchas fire raged, Laboratory crews installed 600 feet of water diversion barriers and removed sediment in anticipation of flash flooding to prevent disruption of trace levels of contaminants in canyons across the Lab's 36-square-mile property. The Lab also removed 65 containers of waste soils and debris from environmental investigation sites in canyon bottoms. Wells in canyon bottoms were sealed, storm water samplers were placed along Lab boundaries, and fish samples from reservoirs and rivers near the fire were tested.

"We routinely collect fish and other species in the Rio Grande both upstream and downstream of the Laboratory and analyze them for radionuclides, metals, and organic compounds," said Chris Echohawk, Los Alamos environmental surveillance program scientist. "There was no increase in radionuclides in fish after the Cerro Grande Fire, but we wanted to collect the samples both before and after any flooding events to assess chemicals such as mercury and polychlorinated biphenyls. We expect to measure fire products similar to any western forest fire."



This photo of the Las Conchas fire, captured at its origination site within an hour of its eruption, reveals how quickly it exploded in this remote forest popular for hiking, camping, fishing, and rock climbing.

Background photo: Gila, New Mexico, hotshots hike into the Valles Caldera to protect this 89,000-acre preserve. CREDIT: KARI GREER/U.S. FOREST SERVICE



Los Alamos residents watch flames approach a few hours after the fire started. The fire reached the hillsides of the town, but homes were spared. Sadly, 63 homes were lost in surrounding communities. CREDIT: JACQUELINE A. SHEN



Santa Clara Pueblo volunteers fight the Las Conchas Fire, which charred more than 16,000 acres on the reservation, nearly half their watershed, and destroyed cultural sites and forest resources. Wildfires have burned two-thirds of Santa Clara's forest over the past 13 years. CREDIT: NATIONAL INTERAGENCY AREA COMMAND



The Laboratory developed agreements with the United States Forest Service, National Park Service, Los Alamos County, and the State of New Mexico to improve emergency response. Here, New Mexico Governor Susana Martinez updates citizens at a press conference in Los Alamos. The Las Conchas Fire was the nation's top-priority blaze at the time, and crews responded from across country. CREDIT. KEVIN ROARK, LOS ALAMOS NATIONAL LABORATORY



Los Alamos National Laboratory Director Charles McMillan, at left, and Senator Tom Udall, second from left, hear an update from a Laboratory environmental specialist during a fire briefing in the Lab's Emergency Operations Center.

CREDIT: JAMES RICKMAN, LOS ALAMOS NATIONAL LABORATORY



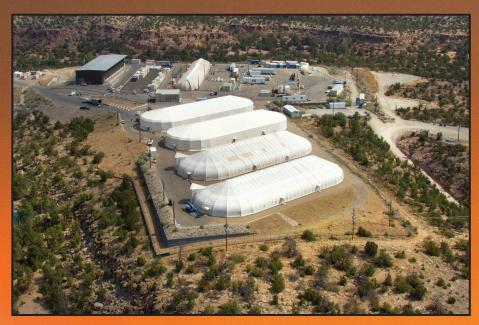
### "I'm happy to live here, happy to breathe the air."

Andrew Green, Environmental Data and Analysis physicist at Los Alamos, commenting on the results from both the Cerro Grande and the Las Conchas fires that revealed no radiation concerns.

A major area of public concern was Area G, a 63-acre site that stores containers of transuranic waste awaiting transport to the Waste Isolation Pilot Plant in Carlsbad, New Mexico. It is the site of the Laboratory's only active disposal pit for low-level waste, such as clothing or tools contaminated by exposure to radioactive materials. However, Area G is paved, ground fuels have been removed, and its metal storage containers have been tested to withstand jet-fuel fires. Daily inspections are made at the site, which is surrounded by groundwater monitoring wells, air-monitoring stations, sensors, and radiation alarms.

LANL also installed more than 60 air monitors throughout the region—even as far as Santa Fe—with a greater concentration near residential areas and cleanup sites. Samples are collected around the clock, and analyzed every two weeks. Samples are independently analyzed offsite to look for dust, smoke, and radioactive particles. According to the New Mexico Environment Department, data around the region revealed no significant radiological detections; minor chemical detections were measured to include ozone, formic acid, smog, methanol, and ammonia—consistent with results normally found in natural fires.

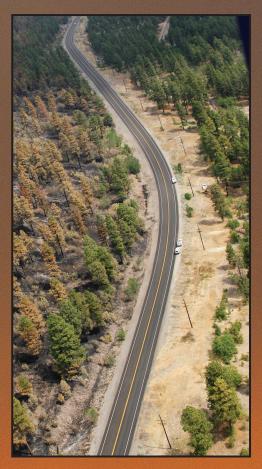
The fire encroached on Technical Area 49, a small parcel of Lab property on the southwest perimeter that hosts facilities used to train military personal to recognize and neutralize homemade explosives (IEDs). The Laboratory had made the affected



Above: Area G contains stores of transuranic and low-level wastes. The area is well fortified against fire: the ground is paved, there are large firebreaks surrounding the buildings, and there are no forests to burn.

Top Right: Clear-cutting along Highway 4, the Laboratory's southern boundary, helped prevent the fire from jumping the road and burning Lab property.

Bottom Right: A worker checks one of the 60-plus air monitors that routinely check air quality. CREDIT: LOS ALAMOS NATIONAL LABORATORY











Top left: The Las Conchas Fire destroyed 63 homes, including this residence overlooking the Valles Caldera. CREDIT: ANONYMOUS PER REQUEST OF THE PHOTOGRAPHER

Bottom left: Los Alamos volunteers helped fill more than 60,000 sandbags at Santa Clara Pueblo to protect against post-fire flooding. The Laboratory donated \$50,000 to a challenge fund to reimburse area businesses that provided goods and services during fire. Support during the fire was widespread—including hotel and dining discounts for evacuees, free housing for displaced pets, and free food for firefighters CREDIT: LOS ALAMOS NATIONAL LABORATORY

Above: A crewmember from ZigZag, Oregon, hotshots guards a burnout in Los Alamos Canyon. CREDIT: KRISTEN HONIG/U.S. FOREST SERVICE

area less vulnerable to fire by removing trees and combustible loads to create fire breaks. The Lab increased monitoring and built the new interagency fire center nearby. Technical Area 49 was designed to withstand fire and was not vulnerable according to Laboratory experts. The fire was stopped nearly half a mile from its well-protected grounds.

By August 2, when the fire was contained, it had charred 156,000 acres in the Jemez Mountains. A million years ago, these peaks were created by a volcano, and the Valles Caldera sits at the center of its collapsed crater. But just as a violent volcano spawned a range of majestic peaks and a pastoral preserve within them, this fire erupted as a reminder of beauty within each beast—of the graciousness of the communities that bonded in support of each other, of the heroic efforts of the 2,000-plus firefighters and aerial support attacking flames in these high-altitude mountains, of our strength, and of the life that will spring from the blackened soil. ❖

"Never again in our lifetime will we see our traditional and treasured homeland and spiritual sanctuary... as we have known it.

It will take generations for our community and lands to recover from the devastation of this fire.
But this is our only homeland; it is the place we have been entrusted with since time immemorial."

Walter Dasheno, Santa Clara Pueblo governor

-Kirsten Fox

## SPOTLIGHT

### **View from the Core**

Making advances in fusion technology—whether for weapons or power production—sometimes requires staring straight into the heart of the matter, into the core where nuclear reactions actually take place. But there's no way to build a viewport into such an extreme environment, unless it's a viewport for neutrons.

Because neutrons are electrically neutral, they are neither attracted nor repelled by the charges of the electrons and the nuclei that surround them in a nuclear reaction. So in some applications, neutrons can fly in straight lines out of the nuclear core, carrying with them valuable information about the conditions inside the core. By allowing the streaking neutrons to hit a position-sensitive detector, researchers can obtain an image of where the neutrons were produced. (In contrast, x-rays and other types of light offer only indirect information about the core because their electromagnetic nature causes them to repeatedly bounce among charged particles before emerging.)

Neutron imaging is important to our national interests. For example, the Los Alamos National Laboratory is tasked to guarantee a test-readiness posture for the nation's nuclear weapons. The Lab uses experimentation and hydrodynamic computer simulations to predict the behavior of those weapons as they age, since they can't be stamped with a simple shelf life. And ever since our voluntary cessation of nuclear testing in 1992, these experiments and simulations have become important substitutes. Being able to see into the nuclear core during experiments,

and using the resulting data to improve the computer simulations, would go a long way toward mastering that mission.

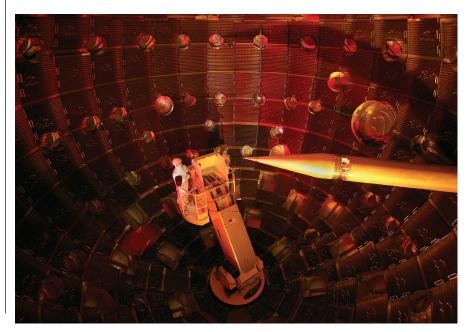
Meanwhile, neutron imaging can also help our country and others to explore the promise of fusion as a power source. To make it work, a region of nuclear fuel as hot as the center of the Sun needs to be created and contained, without consuming more power in that creation and containment than the fusion reactions ultimately deliver.

That's what researchers are trying to achieve at the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory in California. In the facility's target chamber, an incredibly powerful and coordinated blast from 192 ultraviolet lasers converges on a centimeter-sized container that surrounds a millimeter-sized nuclear fuel target. The lasers strike the container and induce it to emit x-rays. These cause the fuel target's outer coating to explode,

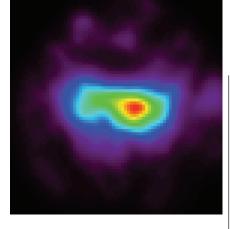
making the fuel itself implode in recoil.

Implosion is the key to inducing fusion, but getting it to happen just so means being able to see what's happening in the core. Fortunately, the fuel is a mixture of deuterium and tritium—both isotopes of hydrogen—and when they fuse together, they produce helium nuclei and spare neutrons. Scientists from the Los Alamos and Lawrence Livermore national laboratories are collaborating to capture the needed visual information from these escaping neutrons.

"Because the neutrons were all produced by the same fusion reaction, they always have the same energy," notes Gary Grim, a Los Alamos scientist on the neutron imaging team. That energy is 14.1 megaelectronvolts, or MeV, a unit of energy commonly used in nuclear physics. A neutron that scatters off of a nucleus on its way out of the core loses energy. The team is able to distinguish between the 14.1-MeV and lower-energy, slower-moving neutrons. This allows them to distinguish between what's happening inside the core and what's happening just outside of it, where scattered neutrons emerge from collisions with nonreacting deuterium and tritium. In other words, discriminating between the neutron energies allows researchers to



In this target chamber at the National Ignition Facility for fusion energy research, 192 ultraviolet lasers converge to deliver two million joules of energy to a nuclear fuel capsule in billionth-of-assecond blasts. CREDIT: LAWRENCE LIVERMORE NATIONAL LABORATORY



An imploding deuterium and tritium fuel target undergoes nuclear fusion and produces neutrons, which have been used to construct this image. Red indicates the greatest intensity of neutrons, while blue and violet indicate the least. Although this image comes from an experiment designed to test the neutron imaging system itself, future images from fusion ignition experiments will be used to assess the degree of desirable spherical symmetry present in the implosion.

identify the size and shape of the core by observing its boundary.

Knowing the shape of the core, among other things, is critical because controlled nuclear fusion as a power source is extremely difficult to achieve. To succeed, NIF will need to perform a number of tasks with virtually no room for error. For example, the laser pulses must be perfectly timed to drive the implosion, and the target must be flawlessly constructed according to a precise design. In addition, the laserinduced implosion must have exquisite spherical symmetry; if the hydrogen isotopes are compressed nonspherically, then the temperature and density conditions needed for fusion will be compromised as nuclear fuel squeezes out of the imploding core. Any departure from the intended spherical implosion provides the fuel with a point of escape.

That's where visualization comes in. This February, the neutron imaging team made their first successful image (shown) of a nuclear fusion experiment, revealing an implosion that was somewhat nonspherical by design, in order to evaluate the performance of the neutron imaging system. This particular image was constructed by observing only the 14.1-MeV neutrons

produced in the core. Researchers will be using imagery like this from future experiments to improve the spherical shape of the imploding target. In the meantime, this successful neutron image demonstrates a critical capability along the road to fusion energy and a proof-of-concept for observing the behavior of nuclear weapons. ❖

—Craig Tyler

### **Uranium Made Easy**

"Uranium possesses a lot of unique properties and has been shown to catalyze reactions that no other element can," says Jaqueline Kiplinger of the Los Alamos Materials Chemistry group. Unfortunately, the processes established more than 20 years ago for getting uranium into a workable form are difficult to carry out, low yielding, and hazardous. Some involve the input of mercury iodide and, therefore, the output of toxic waste.

Kiplinger and her research team recently discovered a better way.

Uranium comes in six oxidation states. U(VI) is the most common in nature and in nuclear fuel processing, while U(III) and U(IV) are often the most useful in the laboratory. The traditional method for reaching the U(III) state leads to a compound called uranium triiodide tetrahydrofuran, but tetrahydrofuran is a finicky ring-shaped molecule that breaks open all too easily during the painstakingly slow, low-temperature production process, leaving behind a radioactive green sludge. And the traditional method for producing U(IV), in the form of uranium tetrachloride, is outright dangerous.

Kiplinger's new process mixes uranium metal shavings with iodine in a dioxane solvent. The resulting U(III) and U(IV) materials are  $\mathrm{UI}_3$  and  $\mathrm{UI}_4$ , respectively, with bound dioxanes. Both serve as precursors to new reaction catalysts, specialty materials (including superconductors), and advanced nuclear fuels.

Compared to traditional methods, the new dioxane method is substantially faster, cheaper, safer, and friendlier to the environment. Moreover, it generates greater than 90 percent yields that can be stored at room temperature—a significant improvement over the earlier 10–20 percent yields that had to be stored cold. Kiplinger expects these benefits to make uranium chemistry much more accessible to government, industry, and university laboratories around the world, enabling more research toward a variety of new applications.

She would know. Her team recently discovered a novel purification process that uses uranium and thorium materials to break apart troublesome contaminants found in natural petroleum reservoirs.



Uranium metal shavings

This type of chemistry was not previously known for any metal in the periodic table. But once Kiplinger's team demonstrated it with uranium, they began trying to engineer substitute materials, using nonradioactive lanthanide or transition metals to mimic the uranium-based chemistry. "Uranium is too radioactive for widespread commercial use," she notes. "But once you learn how to do something with uranium, it's usually possible to find a less dangerous element to do the job instead. Uranium teaches you what's possible." \* LDRD

—Craig Tyler

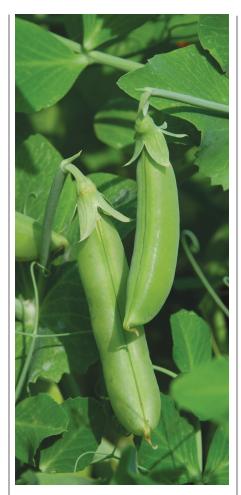
### **Growing Science**

Pat Unkefer of the Bioscience Division knew she needed help getting her discovery "out there." She and her team had discovered that a natural plant metabolite, 2-oxoglutaramate, when applied to plants, stimulates growth by 10 percent or more. Treated plants increase their rates of photosynthesis—they grow faster, get bigger, and mature sooner. The metabolite modifies the plant's metabolism by increasing the amount of carbon dioxide the plant takes from the air and converts to carbohydrates. It also increases the amount of nitrogen the plant takes from the soil. Both processes benefit the environment. Nitrogen is a major pollutant when it washes into waterways, so more nitrogen in the plants means less nitrogen in the soil and waterways. Because carbon dioxide is a greenhouse gas, using the metabolite is also valuable for increasing carbon capture and sequestration.

The metabolite works on all the major crop species and many other species. Its chemical analog can be cheaply manufactured via biosynthesis. It's also biodegradable, meaning this product is relatively environmentally clean to make and to use, and can be certified for use in organic farming.

Could using this product bring about a new agricultural revolution? Would it help feed a starving planet? Would it propel an increase in biofuel production, thus reducing reliance on fossil fuels?

Unkefer thinks so. But where does a Lab scientist go with a promising product? Navigating the world of product development requires a skill set most scientists don't have. Furthermore, it's often a lengthy process requiring lots of determination and hard work. "It's not a path for the faint of heart," says David Pesiri of the Technology Transfer Division (TT), who's working with Unkefer. "The scientists have to passionately believe in their product. It's their passion, their desire to get their product into the hands of people



who can change the world with it, which carries them through the laborious process of licensing and marketing. Passion is a key to moving technologies from the Lab to the marketplace."

Working with the staff at TT is like getting engaged. "Really, we need to believe in the scientist's passion as much as we believe in their product," says John Mott of TT, who also helped Unkefer. "It's going to be a long-term commitment. To be successful will require honest communication, a bit of art, lots of luck, and good timing. We're certainly codependent."

In 1998, with the help of TT and the Lab's intellectual property group, Unkefer patented her product, now called Take-Off. Pesiri and his team then searched for companies that might be interested in licensing Take-Off. They also did the

research required to see which companies met federal and Lab requirements for partnering with the Lab. Companies that will benefit society and the U.S. economy are preferred.

By 1999, 105 companies were contacted. Nine companies expressed interest. A lengthy dialogue ensued to determine which of these suitors met additional requirements. A mature business plan, talented company management, and evidence of enough working capital to nurture the product to success are generally required. These companies, in turn, want additional assurance that the product is all that it's supposed to be. An on-going dialogue with the scientists is key to keeping the prospective companies interested.

Eventually, the Lab reached an agreement with a major U.S. company. However, in 2002, the agreement was mutually terminated due in part to a change in the company's financial outlook. The licensing process had to start over.

In 2003, a new licensing agreement was completed with Biagro Western, a small California-based bioresearch and manufacturing company that sells its products domestically and internationally. Biagro developed Take-Off for the marketplace. Now, Take-Off is available and starting to make a difference. Take-Off is increasing yields in grains and fresh vegetables, while increasing farmers' profitability and helping small farms stay competitive with larger ones.

"Transferring our science to the right licensees is hard work, but when we're successful everybody wins," says Pesiri. "The licensing of Take-Off is a great example of how TT, intellectual property, and Lab scientists can team up and make the world better." \* LDRD

-Clay Dillingham

### Megadroughts of the Southwest

Are you concerned about drilling in the Valles Caldera National Preserve? Don't be: researchers there were drilling for scientific core samples, not for oil. A broad collaboration of university and government organizations, representing the U.S., Australia, and the Netherlands, extracted an 82-meter-deep core from the region. The core contains sediment layers that were deposited between 368,000 and 552,000 years ago, within a 2.6-million-year epoch known as the Pleistocene. Included in the data between these bounding years are two distinct interglacial periods—relatively warmer periods that occur between ice ages—which shed some light on the Holocene interglacial in progress today.

Within the core samples, researchers look for bits of pollen and plant matter, major elements, trace elements, isotope ratios, and other measurables that can

be combined to reveal temperature and aridity. With this information, Los Alamos National Laboratory scientists and collaborators were able to reconstruct an accurate climate history of the Pleistocene

interglacials in the American Southwest. They found that as the interglacial periods progressed, temperatures warmed and brought about wet conditions and plentiful plant life. But continued warming sometimes led to much drier conditions, accompanied by a major decrease in plant life. Such "megadrought" periods occurred at least once in each interglacial, and lasted for hundreds of years—sometimes thousands.

The megadroughts in the study period involved a consistent set of environmental changes. Average temperatures were as high or higher than they are today, and as a result, prevailing mid-latitude westerly wind patterns shifted northwards. This led to substantially reduced precipitation in the Southwest. As a consequence of this increase in aridity, there was a shift in the region's ecology. Pollens trapped in the sediment core revealed that during the megadroughts, spruce and fir trees diminished, as did grass-like plants called sedges. Even some of the most drought-tolerant grasses showed evidence of decline. During the same time period, pollen counts from juniper and oak increased.

Interestingly, some of these same megadrought conditions—higher than average temperatures, aridity, and a juniper and scrub oak ecology—characterize much of the American Southwest today as well. But the Southwest is not presently in a prolonged megadrought. Although the symptoms are similar, they differ in severity. Megadroughts probably resembled the dust bowl of the 1930s, only more arid, and lasting much longer.

Similarities between the current Holocene interglacial and the Pleistocene interglacial imply that more megadroughts could loom in our future. In fact, the study, led by Peter Fawcett of the University of New Mexico, is consistent with modeling results from other researchers that suggest the risk of an upcoming megadrought in the Southwest is probably increased by human-induced climate change. Does that mean that global warming is about to send the Southwest into a megadrought, or prevent its current arid conditions from abating? There is no way to know yet. But as the leader of the Los Alamos component of the team, Jeffrey Heikoop, points out, the better we can understand the major natural cycles, including megadroughts, the better we can understand and predict the climate overall. **\$\times LDRD** 

—Craig Tyler



Interesting features in the geological history of the Southwest were unearthed by core samples drilled from the Valles Caldera National Preserve in New Mexico. For example, this section of a core sample (right) covers approximately 4000 years of time and shows evidence for algal blooms (distinctly white layers) among the finely layered lake muds (darker layers). Analysis of other sections suggested that the region had experienced several extended periods of exceptional dryness.

CREDITS: (ABOVE) FRASER GOFF, (RIGHT) PETER FAWCETT

ISSN: 1942-6631

Presorted Standard U.S. Postage Paid Albuquerque, NM Permit No. 532

Address mail to **1663** 

Mail Stop M711 Los Alamos National Laboratory Los Alamos, NM 87545 email: 1663magazine@lanl.gov Tel: 505-667-1447 Fax: 505-665-4408

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Only a few weeks after New Mexico's Las Conchas wildfire, the charred and blackened grasslands of the Valles Caldera National Preserve, encouraged by summer rains, are already returning to a healthy-looking green.



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A U.S. Department of Energy Laboratory LALP-11-019

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